Hysteretic behavior in weakly coupled double-dot transport in the spin blockade regime.

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Double quantum dot systems in the spin blockade regime exhibit leakage currents that have been attributed to the Hyperfine interaction. We model weakly coupled double-dot transport using a rate equation approach which accounts for Hyperfine flip-flop transitions. The rate equations allow us to obtain self-consistently the time evolution for electronic charge occupations and for the nuclei polarizations in each dot. We analyze the current in the spin blockade region as a function of magnetic field and observe hysteretic behavior for fields corresponding to the crossing between triplet and singlet states.

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The Pauli exclusion principle can play an important role[1,2,3,4,5] in current rectification in molecular and semiconductor nanostructure transport. Spin blockade (SB) is one important example which occurs in double quantum dots (DQDs) over certain ranges of gate voltage, external field, and bias voltage. The interplay between Coulomb and SB can be used to block current in one direction of bias while allowing it to flow in the opposite one. Because of this property DQDs can behave as externally controllable spin-Coulomb rectifiers that have potential applications in spintronics[1]. However, spin relaxation processes, induced by spin-orbit or Hyperfine (HF) interactions, produce a leakage current which partially removes SB. Recently, striking features have been observed in tunneling spectroscopy experiments in both lateral and vertical DQD's[1], where spin flip is attributed to HF interaction. In particular, hysteretic current behavior as a function of an external magnetic field and current instabilities, including time dependent current oscillations, have been observed. These features were observed in the SB regime, i.e., at bias voltages where the current is drastically reduced.

In this letter, we model recent experimental studies of transport through two weakly coupled vertical QD's[6,7]. These experiments analyze transport through weakly coupled QD's in the spin blockade regime under an external magnetic field (B). In the experimental current versus B curves, two striking features are observed: an step in the current and hysteretic behavior. The current step position depends on the source-drain voltage (V_{DC}). We propose a model based on rate equations which includes a microscopic approach of the Hyperfine interaction[8]. The time evolution for electronic charge occupations and nuclei polarizations in each dot is obtained by means of rate equations which are self-consistently solved. In our model we consider up to two extra electrons in the system. Double occupation is allowed only in the right QD. As well we assume that HF interaction is different for the left and right QD. It would be the case for instance, when the number of nuclei within each dot is different. The DQD is biased by a V_{DC} which brings into resonance the inter-dot two electrons state, with opposite spin for each electron, with the right intra-dot singlet state. In this situation the current flows till the electrons in the left and right QD have the same spin polarization. The current drops until spin flip occurs. Then, just a small leakage current flows.

We consider a Hamiltonian: $H = H_L + H_R + H_T^{LR} + H_{leads} + H_T^{l,D}$ where $H_L(H_R)$ is the Hamiltonian for the isolated left (right) QD and is modelled as one-level (two-level)

Anderson impurity. $H_T^{LR}(H_T^{l,D})$ describes tunneling between QD's (superscript "l" describes leads and "D" QD's)[9] and H_{leads} is the leads Hamiltonian. The present model uses rate equations for electron states occupation probabilities. We neglect coherences (reversible dynamics), which is a reasonable assumption as the dots are weakly coupled. The model includes rate equations also for the mean polarization of the nuclei in each QD[8]. Spin flip is included by means of a microscopic model for HF interaction and finally rate equations are self-consistently solved. Our basis consists of twenty states, but those which mostly participate in the electron dynamics at the SB region are: $|\uparrow,\uparrow\rangle$, $|\downarrow,\downarrow\rangle$, $|\uparrow,\downarrow\rangle$, $|\downarrow,\uparrow\rangle$ and $|0,\uparrow\downarrow\rangle$.

Rate equations for state occupation probabilities ρ_s are:

$$\dot{\rho}(t)_s = \sum_{m\neq s} W_{sm}\rho_m - \sum_{k\neq s} W_{ks}\rho_s \tag{1}$$

where $W_{i,j}$ is the transition rate[8] from state j to state i . The HF Hamiltonian is:

$$\hat{H} = \hat{H}_z + \hat{H}_{sf} \tag{2}$$

where

$$\hat{H}_z = [A\langle I_z\rangle]S_z \tag{3}$$

On the other hand,

$$\hat{H}_{sf} = (A/2N)\sum_i \left[S_+I_-^i + S_-I_+^i\right] \tag{4}$$

is the flip-flop interaction responsible for mutual electronic and nuclear spin flip. A is the average HF coupling constant and the nuclear spin I=1/2. Because of the mismatch between nuclear and electronic Zeeman energies transitions must be accompanied at low temperature by phonon emission. We approximate the electronic sf transition rate as[8]:

$$\frac{1}{\tau_{sf}} \simeq \frac{2\pi}{\hbar}| < \hat{H}_{sf} > |^2 \frac{\gamma}{\Delta E^2 + \gamma^2} \tag{5}$$

where γ is the electronic state life-time broadening which is of the order of μeV, i.e., of the order of the phonon scattering rate[10]. ΔE is the difference between the energy of a state with one electron in each dot with aligned spins ($|\downarrow,\downarrow\rangle/|\uparrow,\uparrow\rangle$)and the energy of a state with one electron in each dot with opposite spin orientation ($|\uparrow,\downarrow\rangle/|\downarrow,\uparrow\rangle$) (see Fig. 1). The latter is *mixed* due to interdot tunneling with the intradot singlet state in the right QD ($|0,\downarrow\uparrow\rangle$). The energy of the *mixed* state is calculated through a *two level system* approach

and depends mainly on the inner barrier coupling term (t) and the right and left dots level detuning (Δ). Detuning, Δ, is defined as the difference between the energy of a state with one electron in each dot with aligned spins and the energy of a state with two electrons with opposite spin orientation in the right QD, ($|0, \downarrow\uparrow\rangle$):

$$\Delta = E_{(|\downarrow,\downarrow\rangle/|\uparrow,\uparrow\rangle)} - E_{(|0,\downarrow\uparrow\rangle)} \tag{6}$$

At $B \neq 0$, ΔE depends on B and on the nuclei spin polarization:

$$\Delta E = E_{(|\downarrow,\downarrow\rangle/|\uparrow,\uparrow\rangle)} - E_{(|\uparrow,\downarrow\rangle/|\downarrow,\uparrow\rangle)} \propto g_e \mu_B B + \frac{A}{2} P \tag{7}$$

Here P characterizes the nuclear spin configuration and is defined by $P = \frac{(N_{1/2} - N_{-1/2})}{N}$, where $N_{1/2}$ is the number of nuclei with $I_Z = 1/2$ and $N_{-1/2}$ is the number of nuclei with $I_Z = -1/2$. We consider a finite nuclear spin relaxation time due to nuclei spin scattering ($\approx$ ms[10,11]). The system of time evolution equations for the electronic states occupations ρ_i and nuclei polarization of the left and right dot is self-consistently solved. From that we calculate the total current through the system which is the physical observable of interest (see ref.[8]).

In Fig. 1 the energy levels diagram as a function of Δ is shown. At finite B the interdot triplet state splits (see bottom panel of Fig. 1). At large detuning, increasing B, $|\downarrow,\downarrow\rangle$ is close to the $|\uparrow,\downarrow\rangle$ but electron-nuclei spin scattering is not efficient because it would imply phonon absorption which has very low probability at low temperature. When $|\downarrow,\downarrow\rangle$ crosses the $|\uparrow,\downarrow\rangle$ ($|\downarrow,\uparrow\rangle$) state, $\Delta E = 0$ and according to eq. (5) spin flip has the largest probability to occur. Now electrons and nuclei spin flip processes takes place through HF interaction with phonon emission. They are favorable at temperature close to 0. This is the physical origin for the current step experimentally observed[6,7]. The calculated current versus magnetic field is presented in Fig. 2 where the current step at different source-drain voltages is shown. As the level crossing occurs the current flows and a finite nuclei polarization is induced (see Figs. 2 and 3). It produces an additional Zeeman term which re-normalizes the energy levels. Increasing further B, the current remains constant due to the interplay between the flip flop processes and spin scattering between nuclei which acts removing the nuclei induced spin polarization. Sweeping B backwards, the current remains finite up to the crossing of the levels which now takes place at lower B than in the sweeping forward case due to the feedback between charge occupation and nuclei spin polarization (see Fig.

4). Therefore the current presents a clear hysteretic behavior. We observe as well how the bistability region depends on V_{DC} (as experimentally observed).

In conclusion we have analyzed charge transport through weakly coupled DQDs in the SB regime including HF interactions and considering phenomenologically phonon emission as dissipative mechanism. SB is removed at triplet-singlet levels crossing, once flip-flop mechanism is assisted by phonon emission. The interplay between HF interaction, nuclei dipole interaction and electronic charge occupation produces bistability in the current as a function of the external magnetic field.

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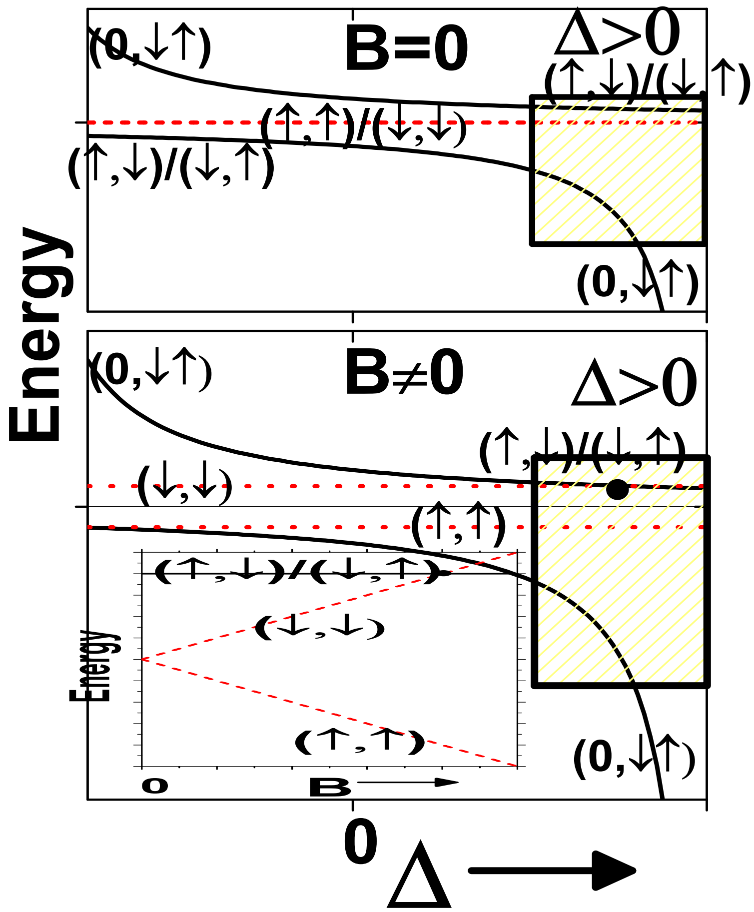
Figure 1. Caption: Bottom panel: Energy levels diagram as a function of the detuning at finite B. At large detuning $|\downarrow,\downarrow\rangle$ is close to the $|\uparrow,\downarrow\rangle$ but electron-nuclei spin scattering is not efficient because it would imply phonon absorption which has very low probability at low temperature. Increasing B, both states cross. As $|\downarrow,\downarrow\rangle$ crosses the state $|\uparrow,\downarrow\rangle$, spin flip flop between electron and nuclei occurs and the current begins to flow. Top panel: same as bottom panel with $B = 0$.

Figure 2. Caption: Current versus magnetic field B. Increasing B, as the level crossing occurs the current flows and a finite nuclei and electron spin polarization is induced. It produces an additional Zeeman term which re-normalizes the energy levels and the current begins to flow. Increasing further B, the current remains constant due to the interplay between the flip flop processes and spin scattering between nuclei which acts removing the nuclei induced spin polarization. Sweeping B backwards, the current remains finite up to the crossing of the levels which now takes place at lower B due to the induced electron and nuclei spin polarization

Figure 3. Caption: Nuclear polarization P versus sweeping up and down B. It can be observed the hysteretic behavior in P giving rise to bistability regions.

Figure 4. Caption: ΔE versus sweeping up and down B at source-drain voltage of 6.6 meV.



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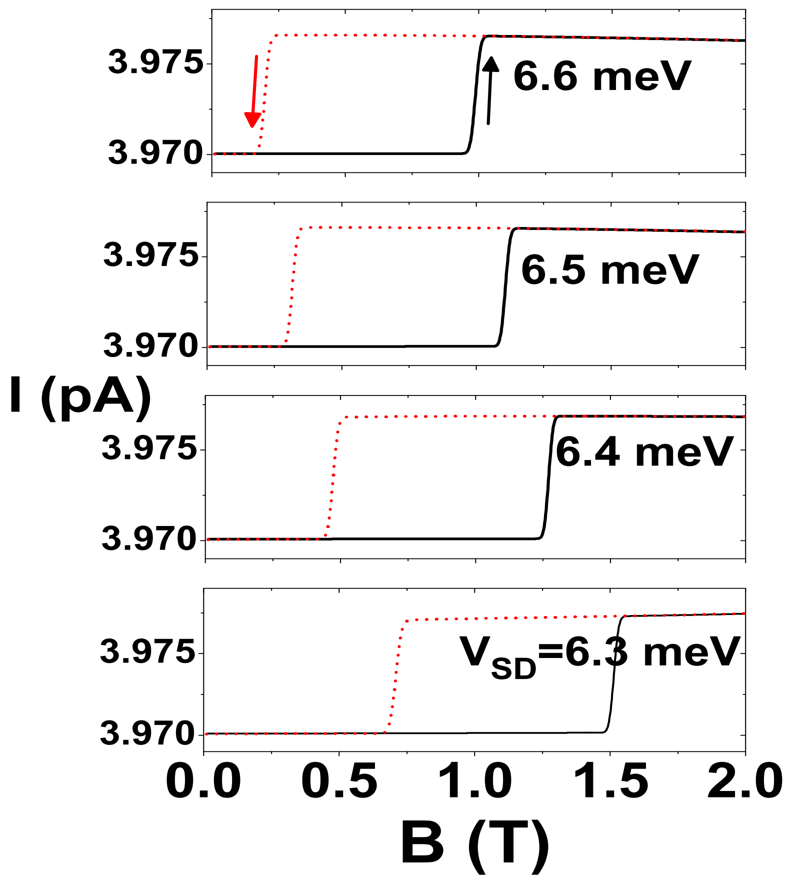

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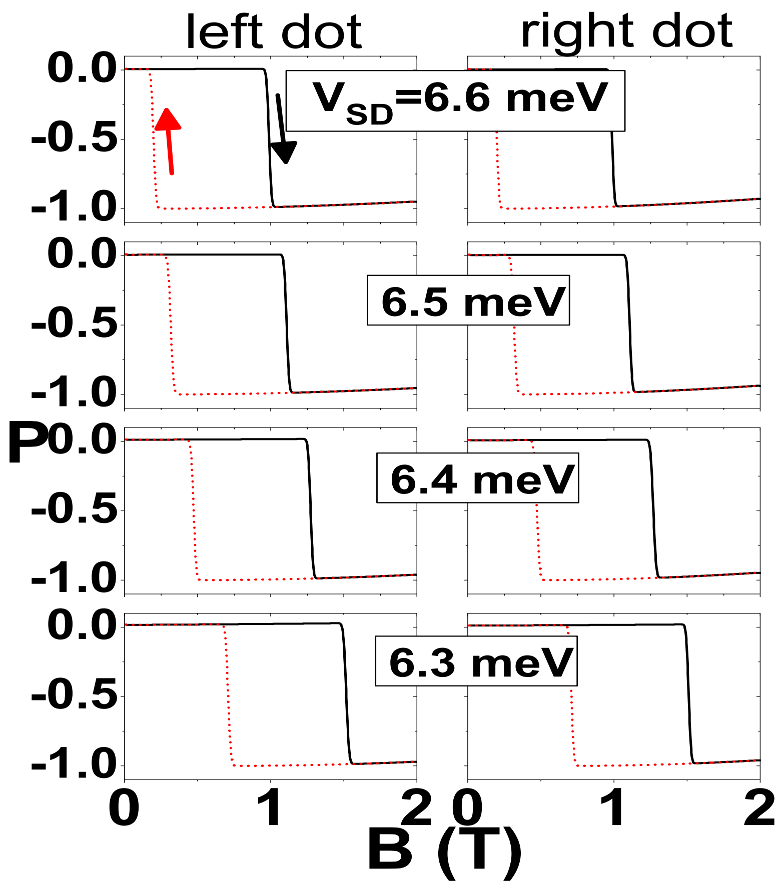

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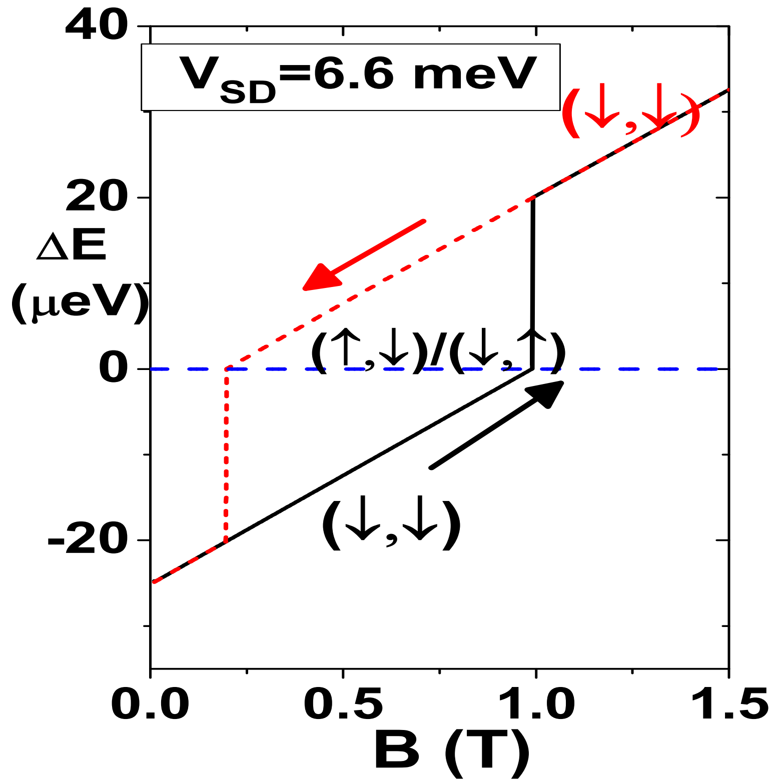

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